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* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2	Apr 08	"Ask CAS" for self-help around the clock
NEWS	3	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS	4	Apr 09	ZDB will be removed from STN
NEWS	5	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS	6	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS	7	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS	8	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS	9	Jun 03	New e-mail delivery for search results now available
NEWS	10	Jun 10	MEDLINE Reload
NEWS	11	Jun 10	PCTFULL has been reloaded
NEWS	12	Jul 02	FOREGE no longer contains STANDARDS file segment
NEWS	13	Jul 22	USAN to be reloaded July 28, 2002; saved answer sets no longer valid
NEWS	14	Jul 29	Enhanced polymer searching in REGISTRY
NEWS	15	Jul 30	NETFIRST to be removed from STN
NEWS	16	Aug 08	CANCERLIT reload
NEWS	17	Aug 08	PHARMAMarketLetter(PHARMAML) - new on STN
NEWS	18	Aug 08	NTIS has been reloaded and enhanced
NEWS	19	Aug 19	Aquatic Toxicity Information Retrieval (AQUIRE) now available on STN
NEWS	20	Aug 19	IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS	21	Aug 19	The MEDLINE file segment of TOXCENTER has been reloaded
NEWS	22	Aug 26	Sequence searching in REGISTRY enhanced
NEWS	23	Sep 03	JAPIO has been reloaded and enhanced
NEWS	24	Sep 16	Experimental properties added to the REGISTRY file
NEWS	25	Sep 16	Indexing added to some pre-1967 records in CA/CAPLUS
NEWS	26	Sep 16	CA Section Thesaurus available in CAPLUS and CA
NEWS	27	Oct 01	CASREACT Enriched with Reactions from 1907 to 1985
NEWS	28	Oct 21	EVENTLINE has been reloaded
NEWS	29	Oct 24	BEILSTEIN adds new search fields
NEWS	30	Oct 24	Nutraceuticals International (NUTRACEUT) now available on STN
NEWS	31	Oct 25	MEDLINE SDI run of October 8, 2002
NEWS	32	Nov 18	DKILIT has been renamed APOLLIT
NEWS	33	Nov 25	More calculated properties added to REGISTRY
NEWS EXPRESS			October 14 CURRENT WINDOWS VERSION IS V6.01, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information
NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that

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specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 17:15:59 ON 01 DEC 2002

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 17:16:05 ON 01 DEC 2002

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 NOV 2002 HIGHEST RN 474744-87-1

DICTIONARY FILE UPDATES: 29 NOV 2002 HIGHEST RN 474744-87-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNnote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> s 4-bromo-2-methoxyestradiol

11862466 4

938248 BROMO

14553906 2

22 METHOXYESTRADIOL

L1

1 4-BROMO-2-METHOXYESTRADIOL

(4 (W) BROMO (W) 2 (W) METHOXYESTRADIOL)

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	16.38	16.59

FILE 'CAPLUS' ENTERED AT 17:16:38 ON 01 DEC 2002

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FILE COVERS 1907 - 1 Dec 2002 VOL 137 ISS 23
FILE LAST UPDATED: 29 Nov 2002 (20021129/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> d ll ibib hitstr abs
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract

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APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS --ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):end

=> d 11 ibib hitstr abs
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:N

=> s 11
L2 2 L1

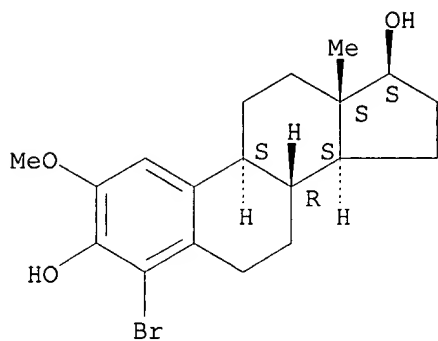
=> d 12 1-2 ibib hitstr abs

L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1989:633338 CAPLUS
DOCUMENT NUMBER: 111:233338
TITLE: Preparations of 2,4-disubstituted estradiols
AUTHOR(S): Pert, Derek J.; Ridley, Damon D.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Sydney, Sydney, 2006, Australia
SOURCE: Australian Journal of Chemistry (1989), 42(3), 421-32
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:233338
IT 97515-50-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 97515-50-9 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 4-bromo-2-methoxy-, (17.beta.)- (9CI)
(CA INDEX NAME)

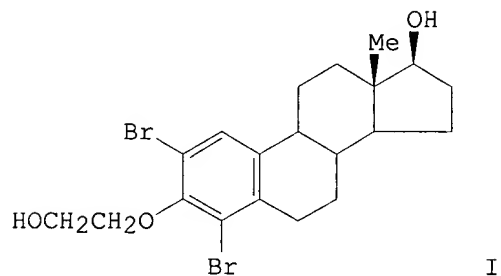
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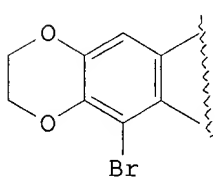
Absolute stereochemistry.



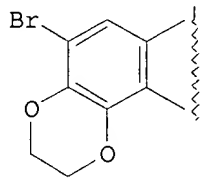
GI



I



II



III

AB Dibromoestradiol I was treated with $\text{CuCl}_2/\text{NaOMe}$ to give [2,3]dioxane II as the major product as well as a minor amt. of the [3,4]dioxane deriv. III. The compds. were used to prep. a no. of 2,4-disubstituted estradiol derivs. Alternative routes to other 2,4-disubstituted estradiols are described.

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:465176 CAPLUS

DOCUMENT NUMBER: 103:65176

TITLE: Catechol formation of fluoro- and bromo-substituted estradiols by hamster liver microsomes. Evidence for dehalogenation

AUTHOR(S): Li, Jonathan J.; Purdy, Robert H.; Appelman, Evan H.; Klicka, John K.; Li, Sara Antonia

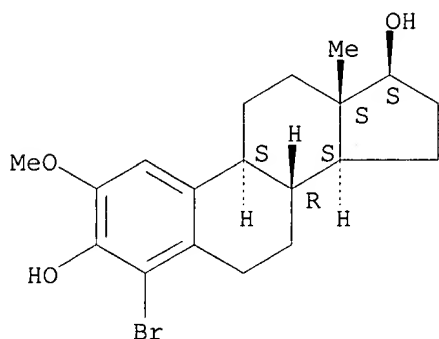
CORPORATE SOURCE: Med. Res. Lab., Veterans Adm. Med. Cent., Minneapolis, MN, 55417, USA

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SOURCE: Molecular Pharmacology (1985), 27(5), 559-65
CODEN: MOPMA3; ISSN: 0026-895X
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 97515-50-9
RL: FORM (Formation, nonpreparative)
(formation of, from halogenated estrogens by liver microsome)
RN 97515-50-9 CAPLUS
CN Estra-1,3,5(10)-triene-3,17-diol, 4-bromo-2-methoxy-, (17.beta.)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



AB Liver microsomes from castrated hamsters were incubated with 2-fluoro-, 4-fluoro-, or 2,4-difluoroestradiols and analogous bromo-substituted estradiols to det. the extent of 2- and 4-hydroxylation with these substrates. Estrogen 2-hydroxylase [9055-96-3] and estrogen 4-hydroxylase [80237-93-0] activity was detd. by radioenzymic assay, and the 3H-labeled monomethyl ether products were identified by HPLC. With unsubstituted 17.beta.-estradiol [50-28-2] as substrate, 97% of the product formed was 2-hydroxylated, and 3% was 4-hydroxylated. The monosubstituted fluoroestradiols exhibited >2-fold enhanced ability to form catechol estrogens compared with their corresponding bromoestradiols. Data presented indicated substantial defluorination when 2-fluoroestradiol [16205-32-6] was the substrate, which amounted to 36% of the total product formed, and 32% of the rate of 2-hydroxylation found with unsubstituted 17.beta.-estradiol as substrate. Interestingly, the rate of 4-hydroxylation was elevated 20- and 6.7-fold, resp., when 2-fluoroestradiol and 2,4-difluoroestradiol [97515-43-0] were the substrates compared to the rate with 17.beta.-estradiol. Moreover, both 4-fluoroestradiol [1881-37-4] and 2,4-difluoroestradiol exhibited at least a 1.6-fold greater rate of 2-hydroxylation compared with 17.beta.-estradiol. In contrast, the rate of dehalogenation with 2-bromoestradiol [15833-07-5] was only 12% of that found with 2-fluoroestradiol. No debromination was obtained with 4-bromoestradiol [1630-83-7] and essentially no catechols were formed using 2,4-dibromoestradiol [19590-55-7] as substrate with these hamster liver microsomes. These data provide evidence for defluorination of these substituted estrogens, particularly at the C-2 position, and seriously hamper the use of fluoroestrogens in studies of hormonal carcinogenicity.